

Advanced Petroleum-Based Fuels Activity

Milestone Completion Report for System Emission Reduction (SER) Analysis, September 2002

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1. INTRODUCTION

The mission of the Department of Energy's (DOE's) Advanced Petroleum-Based Fuels (APBF) activity is to develop advanced petroleum and non-petroleum fuel constituents to enable light-duty vehicles and heavy-duty engines to maintain continuous improvement in engine efficiency and durability while meeting current and planned emission standards and additional potential constraints (e.g. toxins, ultrafine particulate matter (PM), greenhouse gases).

The APBF Program Multi-Year Program Plan (MYPP) outlines research and development needs for advanced petroleum-based fuels for compression-ignition, direct-injection (CIDI) engines for on-road vehicles. The MYPP calls for the development and validation of analysis tools that would be used to set emissions targets for the program and to develop pathways for realizing those targets. Towards that end, the National Renewable Energy Laboratory (NREL) has worked with the Department of Energy on a Systems Emissions Reduction (SER) analysis activity. The purpose of this activity is to analyze the performance of the entire emissions reduction system. SER analysis considers performance of the engine, vehicle, fuel, and aftertreatment devices as an integrated system, including interactions between the system components. The project will develop a "toolbox" of analysis capabilities to assess a variety of efficiency and emissions trade-offs. Three vehicle platforms will be examined: a light-duty passenger car, light-duty truck/SUV, and a heavy-duty engine.

This document is the report for NREL FY 2002 AOP milestone 2.3.1 "Quantify fuel economy penalty associated with various emission control technologies for diesel-powered vehicles" and discusses the progress made towards developing an SER analysis tool. The report includes the following four topics: the SER analysis framework and components in section 2.0, the development of one-dimensional engine models for SER applications in section 3.0, results of quantifying the fuel economy penalties associated with various emission control technologies for diesel-powered vehicles in section 4.0, and future direction in section 5.0. Work was completed in September 2002.

A summary of the accomplishments to date include:

- Developed four WAVE one-dimensional engine models to support SER analysis for the three APBF vehicle platforms. These three platforms are:
 - Automobile class 2.2 liter turbocharged high speed direct injection (HSDI)
 - Light-duty truck/SUV class turbocharged 7.3 liter and a turbocharged 5.0 liter
 - Heavy-duty truck class turbocharged 11 liter
- Performed a simulated assessment of the emissions reduction and fuel economy trade-offs of three diesel engine emissions control technology bundles for the SUV/medium-duty pick-up platform with a CIDI 5.0 liter engine. The technologies evaluated in this analysis included:
 - NO_x adsorber catalyst (NAC) with a diesel particle filter (DPF)
 - Selective catalytic reduction (SCR) with a DPF

- Lean NO_x catalyst (LNC) with a DPF
- Simulated results of the emissions reduction and fuel economy trade-off assessment of three diesel engine emissions control technology bundles for the SUV/medium-duty pick-up platform with a CIDI 5.0 liter engine.
 - For tailpipe NO_x emissions, the NAC at 0.12 g/mile performed slightly better than SCR at 0.13 g/mile over the FTP. The LNC is far behind SCR and NAC at 0.17 g/mile. All three fall short of the Tier 2 Bin 5 goal of 0.05 g/mile—SCR and NAC achieve bin 8, while the LNC achieves Bin 9. SCR, NAC, and LNC, which provided 61%, 63%, and 48% conversion efficiency, respectively, over the FTP, would have to reach 84% conversion efficiency over the FTP to make bin 5. This represents a 38%, 33%, and 75% increase in performance for SCR, NAC, and LNC, respectively, to meet Tier 2 bin 5.
 - For tailpipe PM, the same DPF was used in each technology bundle, so tailpipe results between the three bundles are very close. The NAC/DPF bundle, which, due to the rich spikes increasing engine out PM emissions, had the worst performance at 0.0079 g/mile. The SCR/DPF and LNC/DPF bundles posted 0.0077 g/mile. All technology bundles met the Tier 2 Bins 2 PM limit of 0.01 g/mile.
 - The emissions reductions come with an attendant fuel penalty of up to 2.41% for the NAC, 1.56% for the LNC, and 1.14 % for SCR. This penalty is due to increased backpressure from the catalyst and DPF, additional fuel required for rich-spike regeneration of the NAC, hydrocarbon injection for LNC operation, and fuel necessary for DPF regeneration spread over the number of cycles necessary to fill the filter. Other factors, such as fuel required for NAC desulfation were not included. With the zero sulfur fuel assumed in this study, NAC desulfation events should have a minor additional impact on NAC fuel penalty. The impact on fuel consumption penalty is possibly similar to that of the DPF regeneration, raising the NAC fuel penalty from 2.41% to 2.61%.
 - Reaching higher conversion efficiencies for all three technologies could be achieved by maintaining the exhaust gas temperature at some minimum value using fuel injection into the exhaust gas stream. Urea injection, regeneration of the NAC, and injection of fuel for the LNC were all limited at low catalyst or engine out exhaust gas temperatures. Therefore, raising the exhaust gas temperature would increase urea usage or fuel usage over the values calculated by simulation. The amount of increase is difficult to determine, but may reach 5% or more for the NAC, and 4.5% or more for the LNC. Urea usage for SCR may increase four fold or more. Additional analysis would be necessary to refine these estimates.

2 SER ANALYSIS FRAMEWORK

It is clear that advanced fuels and lubricants, improved combustion, and advanced emission controls will need to be combined in an optimized systems approach in order to meet future vehicle emission standards. Due to the breadth of emission reduction possibilities and complex tradeoffs involved, analysis tools are needed to guide research, evaluate possible emission reduction pathways, and develop optimum technical solutions. The intent of SER is to focus on modeling the entire system in order to understand how the components interact and to provide a framework for optimizing the system as a whole.

NREL has considered several possible directions that could be taken to develop SER analysis tools. The following attributes are considered the basic requirements:

- Ability to accept empirical data relationships being developed in DOE research programs
- Ability to use first principle theoretical models
- Ability to combine empirical models and theoretical models in the same analysis
- Ability to predict both engine exhaust emissions in g/bhp-hr, and vehicle emissions over various drive cycles in g/mile
- Accessible to DOE, national labs, industry, and other stakeholders to promote sharing of information and development of component libraries
- Minimal computer resources needed to perform simulations to allow fast run times on PCs, and to permit rapid evaluations and trend studies
- Hierarchical modeling approaches to allow for development of more sophisticated algorithms if needed
- Leverage on previous DOE research efforts where appropriate
- One-dimensional internal combustion engine model, to allow for more realistic simulation of engine and aftertreatment interaction
- Ability to validate model predictions using APBF program data

Currently NREL is structuring the SER analysis within the framework of the Advanced Vehicle Simulator (ADVISOR) software. DOE, NREL, and industry partners have cooperated to develop ADVISOR for simulating vehicle performance in support of the FreedomCAR initiative and the Hybrid Electric Vehicle Program. ADVISOR is capable of simulating hybrid electric and conventional powertrain configurations and runs in the MATLAB/Simulink environment. Because NREL develops and maintains ADVISOR, the software can readily be modified to accommodate SER analysis features and is easily distributed to DOE partners over the Internet as new versions are released (www.nrel.gov/transportation/analysis).

The ADVISOR software is being enhanced to allow for SER pathway analysis in support of the APBF activity. We envision that these enhancements will also benefit other programs within the Office of FreedomCAR and Vehicle Technologies that perform fuels, emissions, and efficiency analysis.

NREL is currently working on three main enhancements to ADVISOR to improve SER analysis capabilities:

- Addition of component data into the ADVISOR library
- Integration of ADVISOR with an enhanced engine model to allow detailed modeling of internal combustion engines and modeling the interactions with emission control systems
- Development of theoretical and empirical relationships to improve modeling of emission control devices

Collectively, these enhancements will provide the basic capabilities needed to perform SER analysis in support of the APBF program. The goal is to use these enhancements to create an integrated vehicle systems emission reduction model built around the ADVISOR software. The integrated model is composed of three primary components: the vehicle (including the transmission and drive cycle generator), the enhanced engine model, and the emission control system model.

The SER model is currently designed around ADVISOR, but it is also structured to be independent of ADVISOR if necessary. The core structure of the SER analysis is a simple energy and mass balance function between the three system components. The ADVISOR model is used as a drive cycle generator and to account for driveline losses and auxiliary loads, but these functions could be handled through other analytical or modeling methods. Similarly, the engine and combustion modeling will be performed through the use of a one-dimensional engine model, but could utilize a more sophisticated approach in the future. The aftertreatment models can be either empirical relationships or first principle-based models that will also grow in sophistication as the model develops. The critical idea is that the SER analysis is composed of base system components that exchange inputs and outputs to account for system interactions. Low order models and empirical relationships will be used initially with each component growing in sophistication as deemed practical.

It is anticipated that the SER analysis will be used for the following purposes:

- Developing and refining pathways to meet APBF technical targets
- Assessing progress towards meeting the technical targets
- Predicting the effectiveness of new fuel and emission control technologies
- Performing emissions versus energy efficiency trade-off studies
- Working with industry partners to analyze difficult system optimization problems

During FY2002 the focus of the SER analysis work has been concentrated in two main areas. These consist of developing one-dimensional engine models for each of the SER analysis platforms and quantifying the fuel economy penalties associated with various emission control technologies for diesel-powered vehicles. The following two sections detail the progress in these areas over FY 2002.

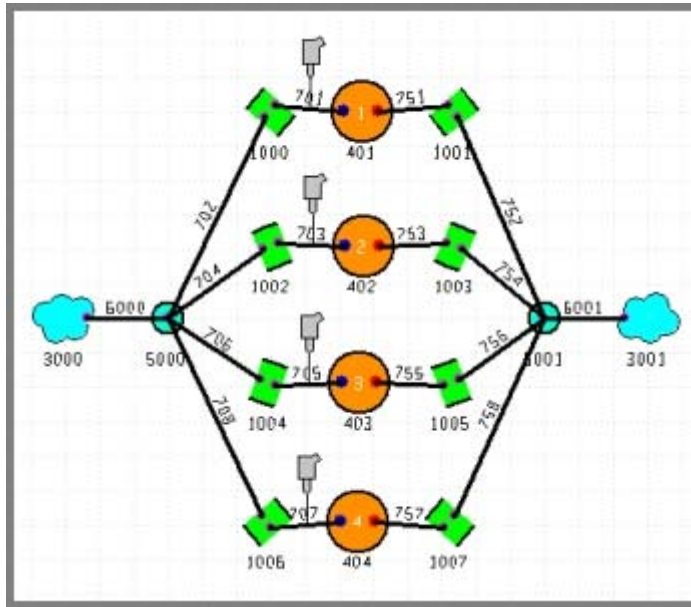
3 DEVELOPMENT OF ONE-DIMENSIONAL WAVE ENGINE MODELS

Under the current SER structure of using ADVISOR as the base framework, it will be necessary to integrate simulation results/data with ADVISOR to perform system level analyses. WAVE one-dimensional engine models will be used to accomplish this task. Efforts this year have focused on developing these models for each analysis platform so that engine simulations could be performed. These models will also have utility as stand alone analysis tools that can be used to perform a variety of efficiency analyses within the SER context.

WAVE is a one-dimensional engine performance and gas dynamics simulation software program. It comes packaged with links to several other popular simulation packages, including MATLAB/Simulink. NREL developed four one-dimensional engine models using the WAVE software during FY2002. The primary objective of this work was to develop detailed, calibrated WAVE engine models (with supporting data) of the following four diesel engine types; intended to match the three SER/APBF analysis platforms.

1. Automobile class 2.2 liter turbocharged high speed direct injection (HSDI)
2. Light-duty truck/SUV class turbocharged 7.3 liter and a turbocharged 5.0 liter model which was scaled-down version of the 7.3 liter model.
3. Heavy-duty truck class turbocharged 11 liter

To date all four of the models have been developed. For illustrative purposes Figure 1 shows the WAVE graphical representation of a generic engine model. The cylinders are represented in orange, fuel injectors in gray, the manifolds and junctions in teal and lime, the connecting pipes in black, and ambient and exhaust air in blue.



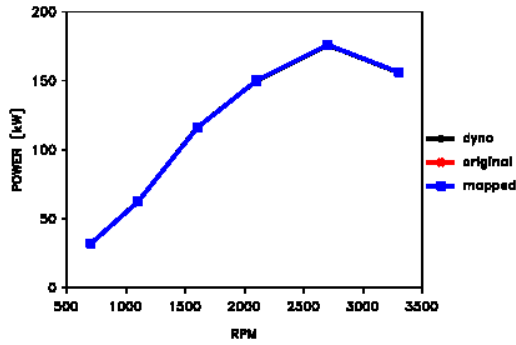


Figure 2: Full-load WAVE-mapped Engine Power vs. Tested Power

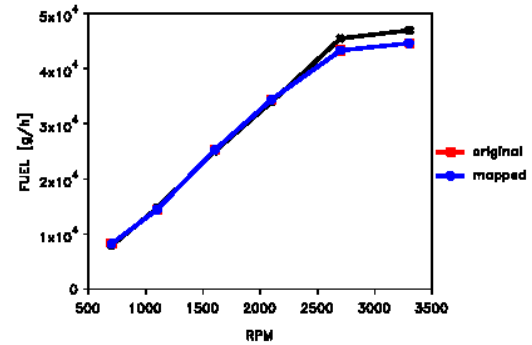


Figure 5: Full-load WAVE-mapped Engine Fuel Rate vs. Tested Fuel Rate

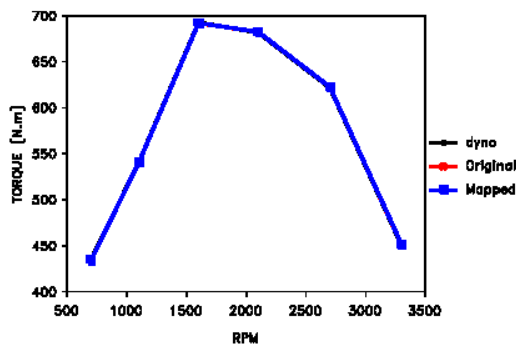


Figure 3: Full-load WAVE-mapped Engine Torque vs. Tested Torque

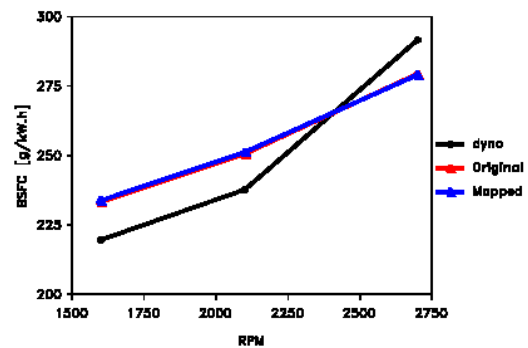


Figure 6: Partial-load WAVE-mapped Engine BSFC vs. Tested BSFC

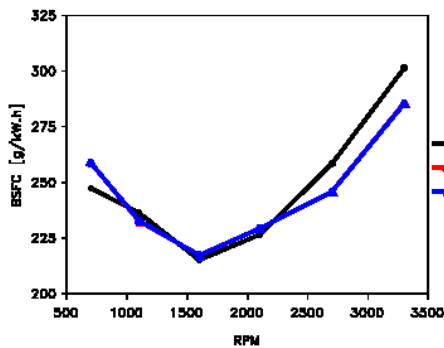


Figure 4: Full-load WAVE-mapped Engine Brake-specific Fuel Consumption (BSFC) vs. Tested BSFC

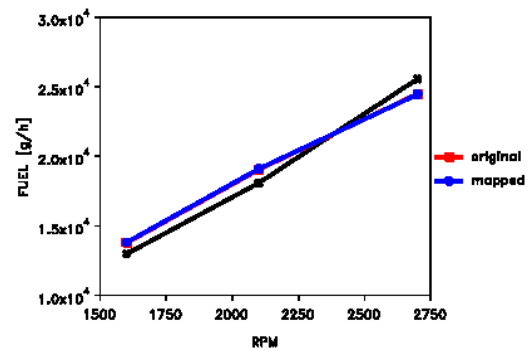
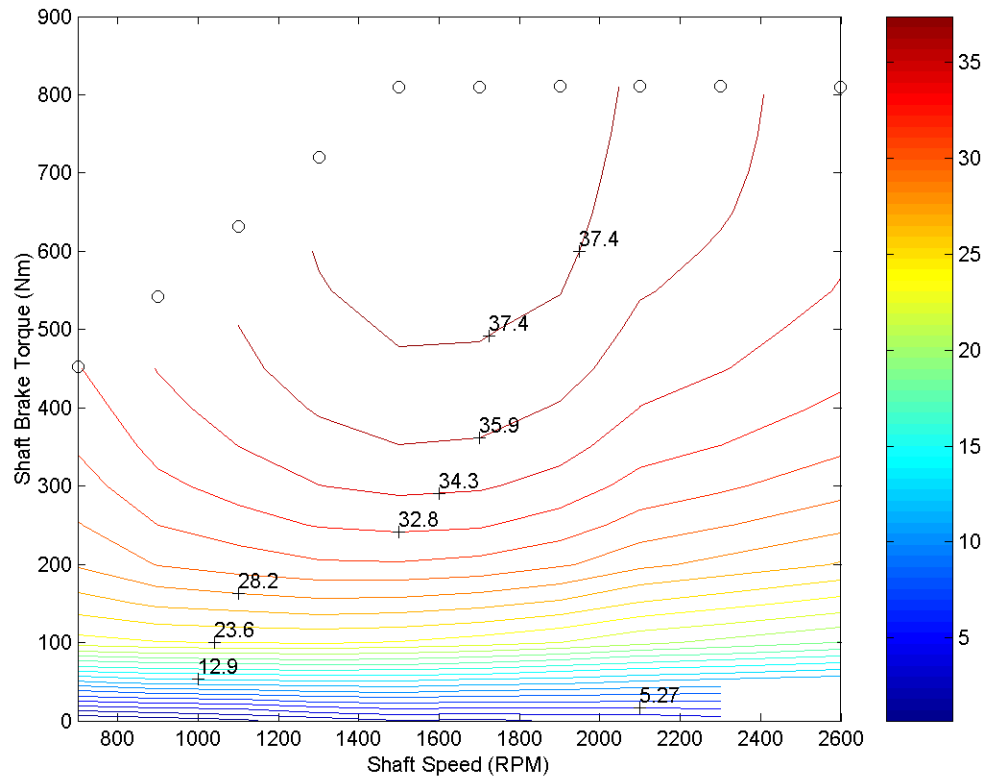


Figure 7: Partial-load WAVE-mapped Engine Fuel Rate vs. Tested Fuel Rate

An efficiency map from the 7.3 liter WAVE engine model is shown in Figure 8. The black circles give the maximum torque generated by WAVE for each speed simulated. For comparison, Figure 9 is an efficiency map created from the original test data.



**Figure 8: WAVE-generated Engine Map Showing Efficiency by Torque and Speed
(Based on International 7.3 liter Engine Model)**

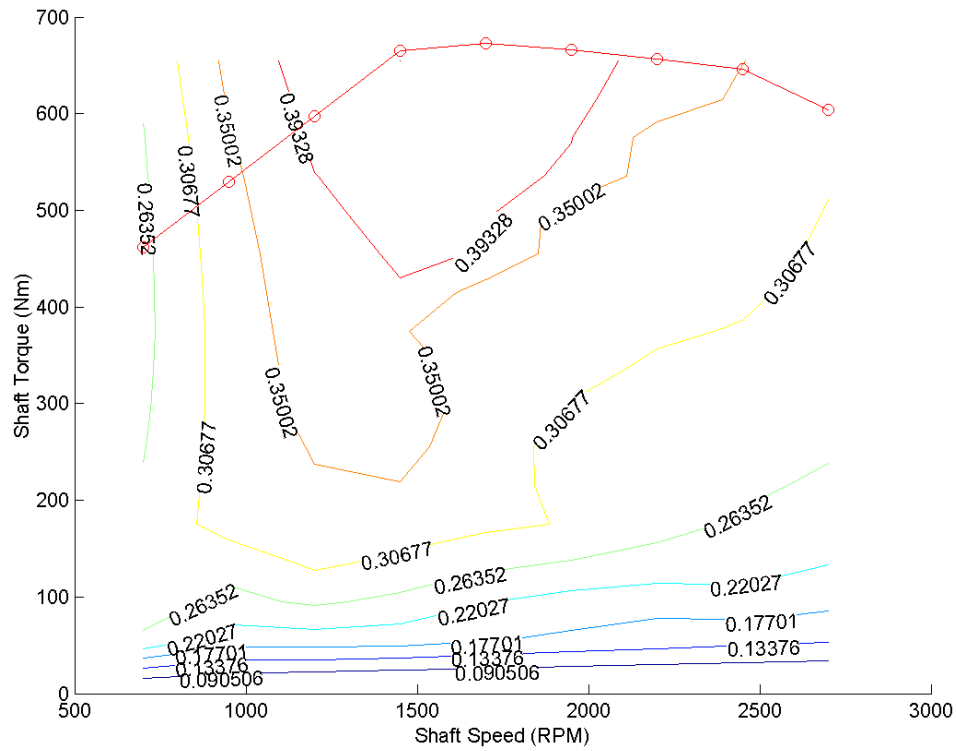


Figure 9: Efficiency Map Generated Using Base Data

The difference between the efficiency maps and maximum torque curves of Figure 8 and Figure 9 is shown in Figure 10. The jagged line for the maximum torque curve occurs because both torque curves are overlaid and points connected. The maximum torque curves differ, but efficiency (expressed as a decimal between 0 and 1) is similar.

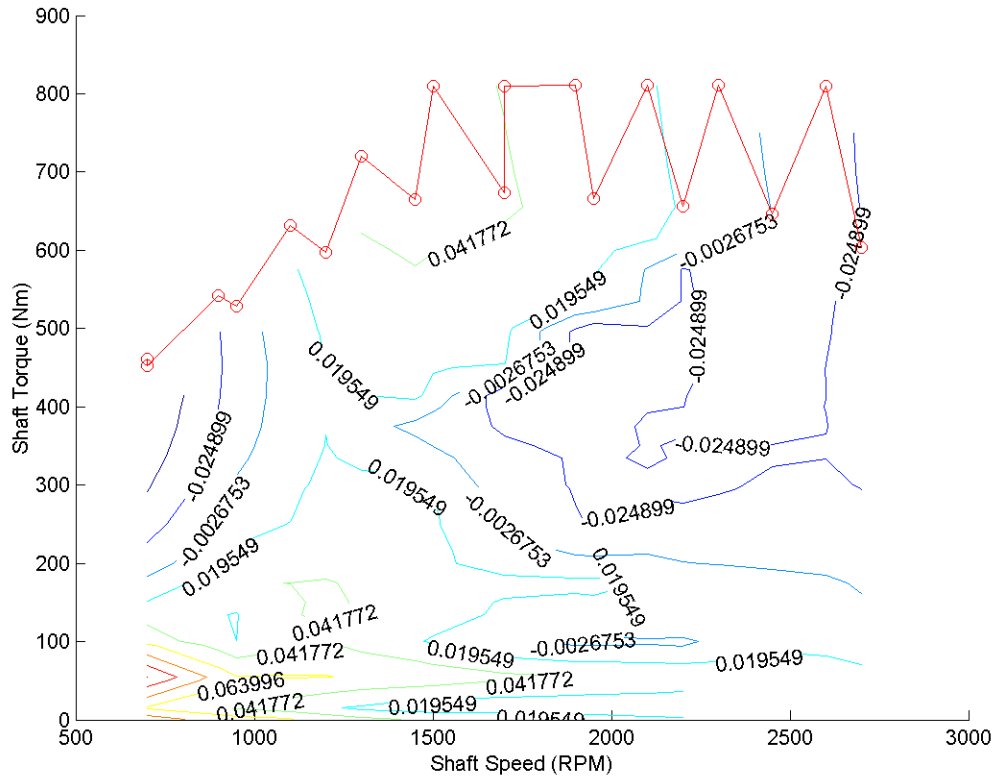


Figure 10: Map Showing Difference Between WAVE-predicted Efficiency and an Engine Map Based on Test Data

Fine tuning may be required to achieve a better match with the test data. Once the model is validated, a wealth of information is available for use in other analyses. For example, Figure 11 and Figure 12 show exhaust temperature and exhaust mass flow by engine output torque and speed. These data can be used in aftertreatment conversion efficiency analyses. In Figure 11, WAVE predicts exhaust temperature to be independent of torque (i.e., loading). These and other results must be validated before work continues.

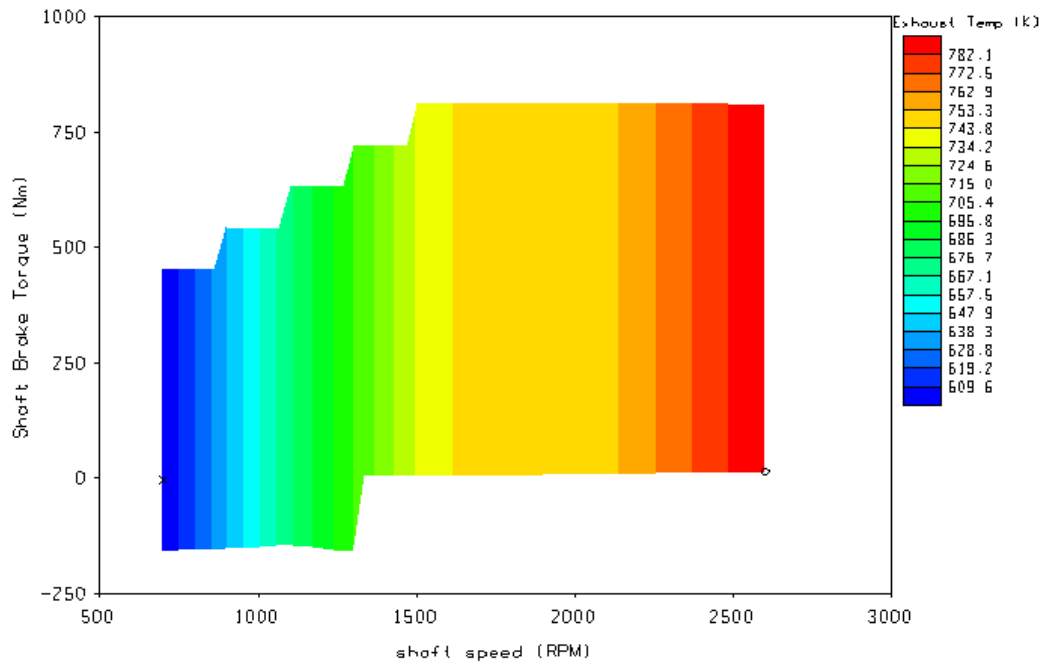


Figure 11: Engine Exhaust Temperature by Shaft Torque and Speed as Predicted by WAVE International Model

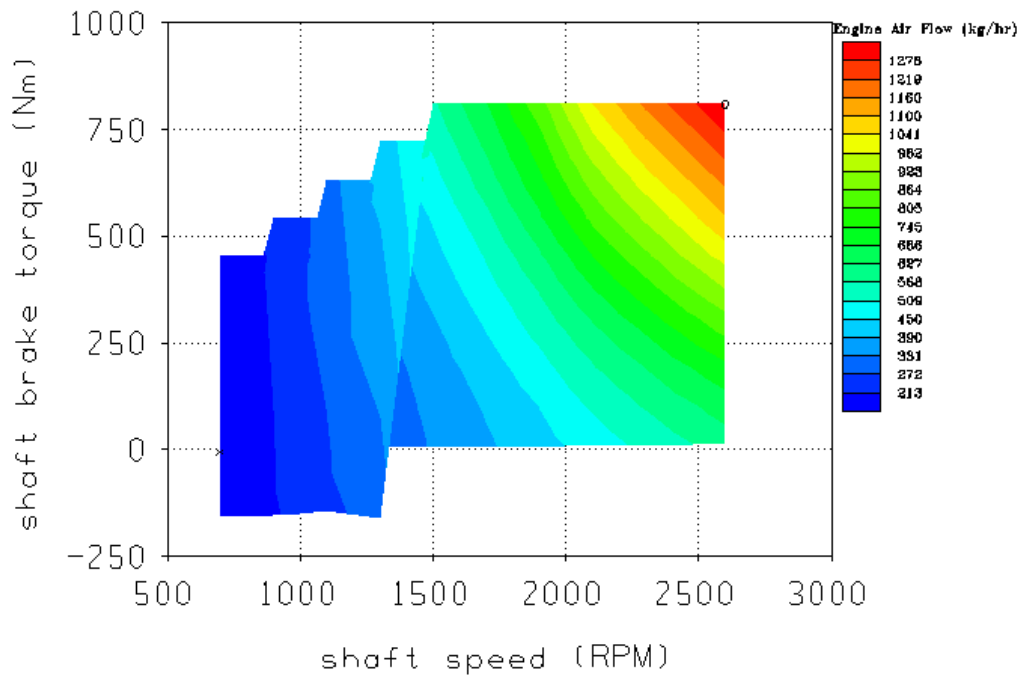


Figure 12: Engine Exhaust Mass Flow Rate as Predicted by WAVE International Model

4 RESULTS OF QUANTIFYING THE FUEL ECONOMY PENALTIES ASSOCIATED WITH VARIOUS EMISSION CONTROL TECHNOLOGIES FOR DIESEL-POWERED VEHICLES

The emissions reduction fuel penalty trade-off analysis for three CIDI emissions control technologies for a single vehicle platform was accomplished in FY 2002 by using engine models in conjunction with emissions control models, other analytical tools, and literature data. The purpose of this was to develop an analysis approach that would allow for a standardized comparison of emerging lean exhaust emissions control technology bundles. This task was completed with assistance from Ricardo Inc. under an NREL subcontract.

The first phase of this effort was to assess the emissions reduction and fuel economy trade-offs of three emissions control technology bundles that are anticipated to be the near term best approach to meeting Tier 2 emissions standards for CIDI applications.

The technologies evaluated in this analysis included:

1. NO_x adsorber catalyst (NAC) with a DPF
2. Selective catalytic reduction (SCR) with a DPF
3. Lean NO_x catalyst (LNC) with a DPF

Each of these emissions control systems will be evaluated for the SUV or medium-duty pick-up platform with a CIDI 5.0 liter engine.

Other emissions control technologies and vehicle platforms will be modeled and evaluated under future tasks in FY03.

For the purpose of this analysis it was assumed that the analysis vehicle will be equipped with state-of-the-art engine technology, including charge air cooler, turbocharger, and EGR. In addition we also assumed that all systems were be used in conjunction with near zero ultra-low sulfur fuel in order to simplify the simulation. Under this assumption, the potential impact of sulfur contamination was not considered in this analysis.

The emissions reduction estimates and fuel consumption trade-offs were calculated in two separate formats. The first format was to report the fuel consumption relative to achieving the Tier 2 bin 5 emission levels (0.07 g/mi NO_x and 0.01 g/mi PM). The fuel consumption change was reported in percent change from a baseline of a current production diesel vehicle for this platform. That is, simulated emissions and fuel consumption baselining was required as part of this effort. The second format was to evaluate the fuel consumption and emissions reduction trade off incrementally, as grams of fuel used per gram of emission avoided. Finally, the above information was also presented graphically showing the maximum simulated reduction capabilities of all three technology bundles and the accompanying fuel consumption increase. To the highest degree possible, all aspects of the emissions control systems were accounted for in this analysis. All reductants (fuel or urea) and all electrical or other engine parasitic load

requirements were converted into equivalent fuel consumption units. This effort required the use of a variety of analysis tools including ADVISOR, WAVE, and MATLAB/Simulink. In some cases it was necessary to utilize a variety of modeling and analytical tools, as well as empirical information and data from published studies in order to fill in gaps in simulation capabilities.

The general technical approach to this task is as follows:

1. Determine engine speed and load points for the vehicle over the FTP
2. Determine engine emissions over speed and load range
3. Use engine speed and load points to access engine emissions maps to determine engine out emissions stream over the FTP
4. Size catalysts based on emissions stream
5. Tune/calibrate emission control models to available data
6. Apply emission control models to emissions stream
7. Estimate emissions reduction benefit and fuel economy trade-off

The general framework for all the emissions control technology models are built around MATLAB/Simulink. These one dimensional, quasi-steady models are designed for an “intermediate level of complexity” and include:

- Mass transfer through the catalyst
- Diffusion of exhaust species to and from the monolith
- Heat transfer between the monolith and the exhaust stream and between the monolith and the ambient
- Global chemical reaction kinetics
- Heat of reaction

The models allow the user to define the number of axial segments the catalyst is divided into. All simulations for this study were performed with 20 to 25 segments.

To determine the mass transfer, a quasi-steady approach was taken. This is the same approach as taken in Oh and Cavendish (1). The basis of this assumption is that the time constant of the thermal response is much larger than the change of gas concentration with respect to time.

Heat transfer was determined based on the methodology outlined by Lubeski (2) with conduction along the monolith and heat loss to the ambient added using a finite difference approach. This model assumes that radiation is negligible.

To simplify the study a model of the heat loss in the pipe up stream of the catalyst is not included. A constant exhaust temperature loss of 10°C was assumed to occur between the turbine outlet and the catalyst inlet. While this number is low when compared with heavy-duty applications experience, this figure is reasonable due to the much lower than usual exhaust temperature over the light-duty test cycle resulting in less heat transfer. Furthermore, it is assumed that conversion efficiency concerns would increase the

priority of catalyst placement and heat loss reduction during vehicle development such that heat loss would be minimized.

Heat transfer between the monolith and the ambient was determined using material thermal conductivities, specific heats, and densities from Chen, Bisset, Oh and Van Ostrom (4).

Vehicle Model

NREL's advanced vehicle simulator, ADVISOR version 3.2 SUV model was used to simulate the vehicle platform. The base model is equipped with a 3.6 liter gasoline engine; the engine model was modified to reflect the 5.0 liter turbocharged diesel. Pertinent details of this model are contained in Table 1.

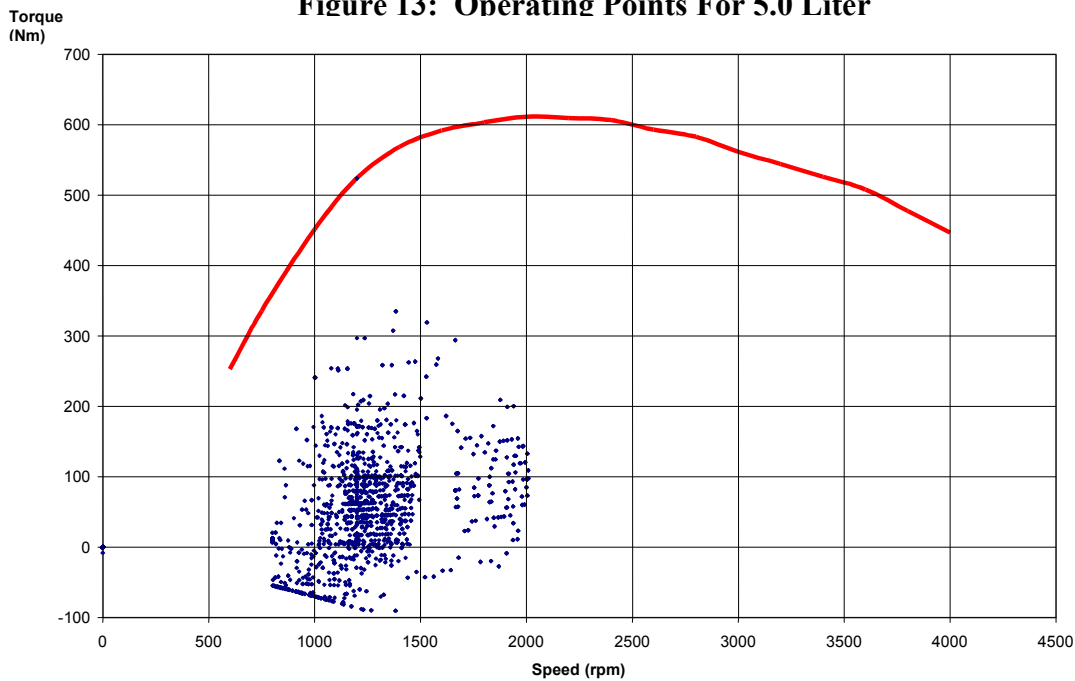
Table 1: SUV model details

File Name	Sport_Utility_in.m
Vehicle Mass	2164 kg
Transmission	Manual 5 Speed
Transmission + Final Drive Ratios	13.45 7.57 5.01 3.77 2.83
Shift Schedule	Advisor default

The vehicle mass of 1949 kg was based on the average of a 1998 Ford Explorer, Jeep Grand Cherokee, and Chevrolet Blazer and includes 300 pounds for cargo. This mass was increased to 2164 kg to account for the larger 5.0 liter diesel engine.

Engine operating points from the FTP drive cycle versus the maximum torque envelope of the engine are shown in Figure 13. As can be seen in Figure 13, the engine is lightly loaded during the FTP, with most of the operating points under 50% engine redline speed and 50% engine peak torque. While modifying gear ratios and transmission shift schedules may result in better utilization of the engine, the values used were considered reasonable.

Figure 13: Operating Points For 5.0 Liter



Engine Model

An engine displacement of 5.0 liters was chosen based on currently available vehicles. As there are no such state-of-the-art 5.0 liter turbocharged diesel engines currently on the market, engine performance and emissions were based on experience with similar engines, research, and the 5.0 liter WAVE model produced for another part of the SER project.

This engine represents an aggressive, yet achievable engine out NO_x value, and has been demonstrated by state-of-the-art engines. Its performance is accomplished through high levels of EGR—approximately 50% at low engine speed/low load operating points.

Figure 13 shows the speed and load envelope for the engine. Peak torque point is 611 Nm (15.4 bar bmep) at 2000 rpm, while peak power is 192 kW at 3600 rpm. Redline is 4000 rpm.

We focused the effort of estimating engine emissions on the areas of the speed load range corresponding to the operating points from the vehicle model. The result was a set of maps, each map representing a specific relevant parameter versus speed and load.

Rich operation was accomplished through a combination of EGR, inlet throttling, injection timing adjustments, pilot and/or post injection, turbine nozzle rack adjustments and increased rail pressure. The rich maps used during regeneration events reflect a relative air/fuel ratio of 0.92. Data were presented as percentage change from lean operation over the range of speed and loads demanded by the vehicle.

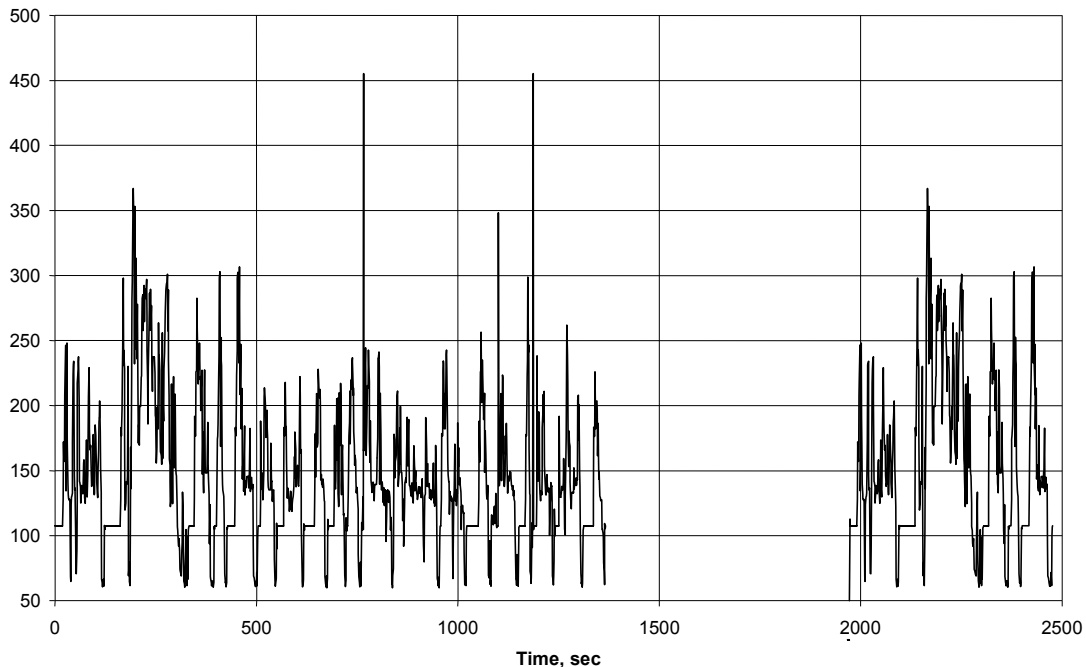
The set of maps was then loaded into a MATLAB/Simulink mapped engine model. This model took the speed and load operating points from the vehicle simulation and accessed the emissions look up tables to determine the engine out emission flow rates, exhaust temperature, exhaust flow rate, and fuel consumption with respect to time over the FTP. Cycle totals were determined by integrating the appropriate values.

The turbine outlet exhaust gas temperature and NO_x and PM cumulative emissions values are presented as Figures 14 and 15. As can be seen from Figure 14, the exhaust temperature is relatively low over the entire FTP. In fact, the exhaust gas temperature exceeds the urea injection threshold of 180°C for only 388 seconds of the FTP. With the cumulative emissions shown in Figure 15, an 84% reduction of PM and 78% reduction in NO_x is required to make Tier 2-bin 5 limits.

To determine the effects of increased backpressure on engine fuel economy, a neural network was built based on WAVE simulations. The neural network characterized brake specific fuel consumption (BSFC) based on engine speed, load, and backpressure. The neural network fit of the data had a maximum error of 3% and an average error of less than 0.5%. The effect of backpressure on fuel consumption is small for this application. The work of Hermann, Lang, Mikulic, and Scholz (7) resulted in similarly small effects of backpressure.

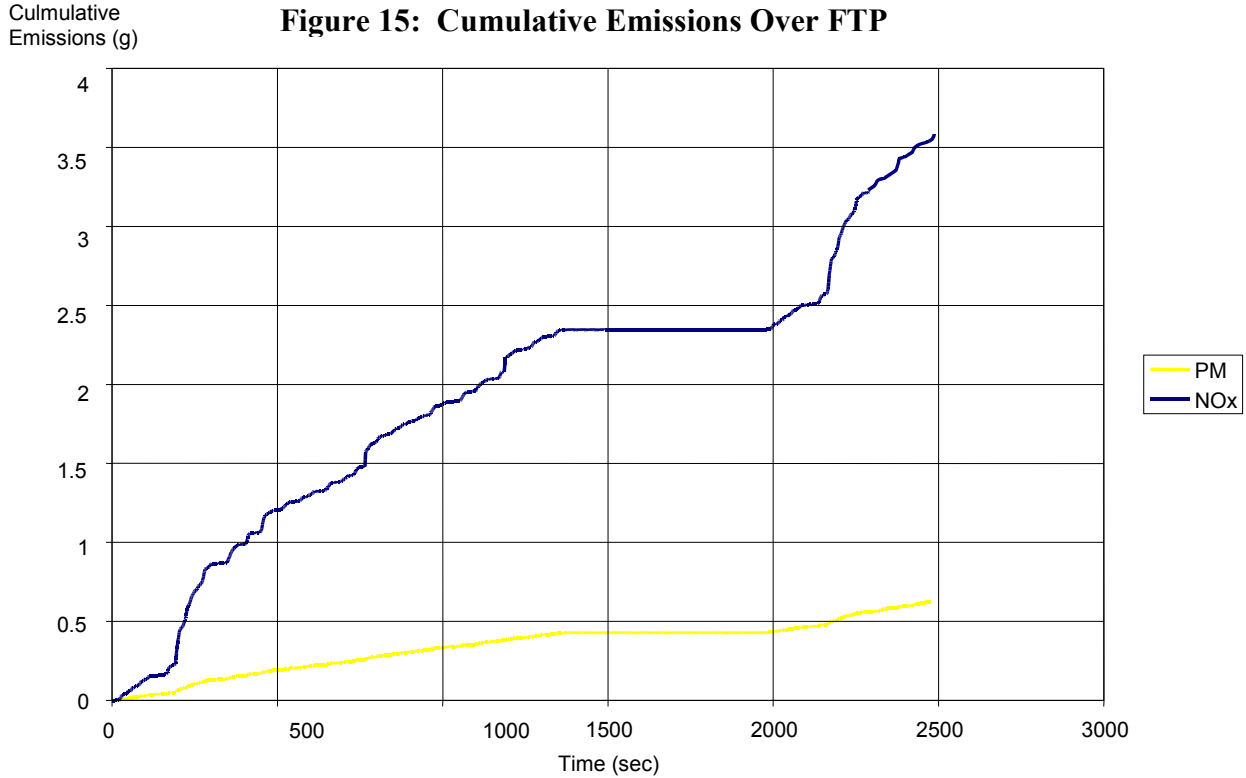
Turbine Outlet
Exhaust Gas
Temperature
(degrees C)

Figure 14: Turbine Outlet Exhaust Gas



The backpressure of the normal exhaust system was assumed to be 9.0 kPa at rated power based on experience with similar engines. As previously discussed, the exhaust was

assumed to be free of sulfur. This precluded the necessity of desulfation of the NAC, and prevented any poisoning of the catalysts.



Emissions Control System Sizing and Layout

The low exhaust gas temperatures, even at the turbine outlet, preclude continuous or even intermittent low temperature NO_x based passive regeneration. Therefore, it was decided that the catalyst in each technology bundle comes before the DPF to allow maximum utilization of the exhaust gas energy. Active (catalyzed) DPF regeneration was initiated by introducing additional fuel upstream of the DPF.

After determining system layout, the individual components needed to be sized. This was accomplished using both published and internal data in combination with the engine out emissions stream discussed previously. The device sizing is itemized below.

- For the DPF, an 8.0 liter silicon carbide (SiC) DPF was selected based on the assumptions of 5 g/L soot capacity and one regeneration per 50-60 FTP cycles.
- A 7.5 liter SCR was selected based on literature review.
- A 5.1 liter NAC was sized based on internal experience, and assumes 2 g/L NO_x capacity and relatively high precious metal loading. The loading and volume of

this catalyst have been increased over normal to deal with the low exhaust temperatures.

- The LNC was assumed to be identical in size to the SCR catalyst.

The following provides a detailed discussion of each individual emissions control component model.

SCR Model

The first of the aftertreatment technology modeled was the urea-based SCR. For this study, a somewhat simplified model was used. A urea solution is injected into the exhaust upstream from the catalyst, which ideally, given sufficient time and exhaust temperature, decomposes to ammonia. The ammonia then reduces the NO_x to N₂ in the presence of the precious metals in the device. Although sources report many NO_x reduction mechanisms, a five reaction set approach was taken to model SCR:

- $4\text{NO} + 4\text{NH}_3 + \text{O}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}$
- $\text{NH}_3 + \text{MO} \rightarrow \text{MO}^*$ (ammonia storage)
- $\text{MO}^* \rightarrow \text{NH}_3 + \text{MO}$ (ammonia release)
- $2\text{NO}_2 + 4\text{NH}_3 + \text{O}_2 \rightarrow 3\text{N}_2 + 6\text{H}_2\text{O}$
- $\text{NO} + \text{NO}_2 + 2\text{NH}_3 \rightarrow 2\text{N}_2 + 3\text{H}_2\text{O}$

More complex reaction sets are difficult to tune, especially given the lack of detail in the data presented in published literature. Likewise, global chemical reaction rate equations are difficult to locate. Therefore, the following rate mechanisms were assumed:

$$R_1 = \frac{A_1 e^{-B_1/T} [\text{NO}] [\text{NH}_3]}{1 + C_1 e^{-D_1/T} [\text{NH}_3]} \quad (1)$$

$$R_2 = A_2 [\text{MO}] [\text{NH}_3] \quad (2)$$

$$R_3 = A_3 [\text{MO}^*] [\text{NH}_3] \quad (3)$$

$$R_4 = \frac{A_4 e^{-B_4/T} [\text{NO}_2] [\text{NH}_3]}{1 + C_4 e^{-D_4/T} [\text{NH}_3]} \quad (4)$$

$$R_5 = \frac{A_5 e^{-B_5/T} [\text{NO}] [\text{NO}_2] [\text{NH}_3]}{1 + C_5 e^{-D_5/T} [\text{NH}_3]} \quad (5)$$

where:

- | | | |
|-----|---|------------------------------|
| R | = | reaction rate (kmol/s) |
| [x] | = | mole fraction of species 'x' |
| T | = | monolith temperature (K) |

To tune the pre-exponential and exponential constants in the rate equations, data from Blakeman, Chandler, John, and Wilkins (3) was used. Catalyst “B” of this reference exhibits very good performance at low temperatures, especially when sufficient NO₂ is present. Blakeman et al (3). reports catalyst “B” results with NO only stream and a 50/50 mix of NO and NO₂, which allowed tuning of both reactions 1 and 5. Reaction 4 was assumed to have the same constants as reaction 1. Figures 16 and 17 show a comparison between the model and the reference data for the NO only and NO+NO₂ tests, respectively.

As can be seen in Figure 16, the model achieves a very good match with the data between 150°C and 275°C. Since there is no NO₂ in the stream, just NO, this result is solely due to reaction 1. Note that the minimum temperature for which Blakeman et al (3) supplied data was 150°C. While the model predicts a constant conversion efficiency decrease with decreasing temperature below 150°C rather than some steep drop off, little importance was placed on this due to urea injection restriction beneath 180°C, which will be discussed in more detail below. The divergence of the two traces above 275°C is also of little importance since the catalyst in this study will rarely, if at all, operate at this temperature.

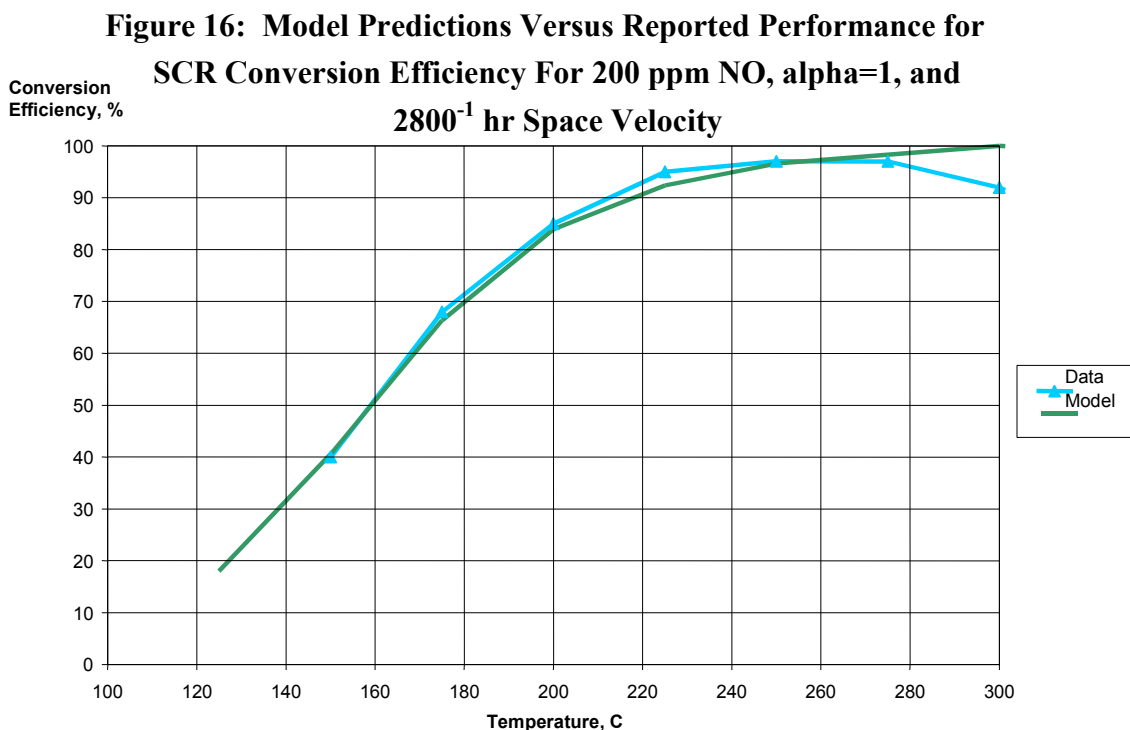
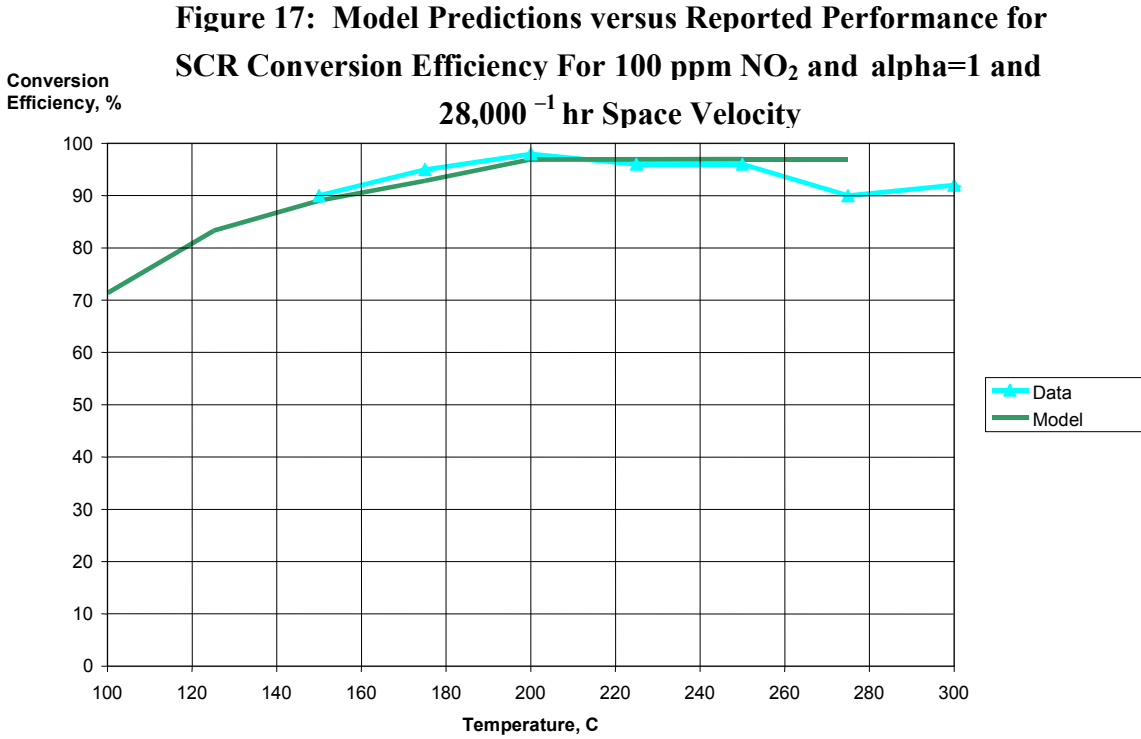


Figure 17 shows a very good match between 150°C and 250°C. Since both NO and NO₂ are present, this result is due to reactions 1, 4, and 5. Once again, low temperature extrapolation and high temperature divergence are considered unimportant due to the operating temperature and urea injection restrictions of this study.

Blakeman et al (3) states that catalyst "B" exhibited minimal ammonia storage. Therefore, constants for reactions 2 and 3 were set to a suitably small value.



To avoid partial conversion of urea to ammonia, which could lead to undesirable byproducts, urea injection was limited to times when the exhaust temperature was above 180°C. When injected, the urea supply was continuous and the flow rate was determined by:

$$\text{mols/s Urea} = \alpha \left(\frac{\text{mols NH}_3}{\text{mols NO}_x} \right) \times (\text{mols/s NO} + \text{mols/s NO}_2) \times \frac{1 \text{ mol Urea}}{2 \text{ mol NH}_3}$$

The ratio of NH₃ to NO_x, α , is dependant on many things, including catalyst formulation, ammonia storage capability, and tolerance to ammonia slip (for example, a catalyst downstream of the SCR catalyst may be able to remove the ammonia). For the purposes of this simulation, α was assumed to equal one. Conversion was assumed to be instantaneous.

For this application, catalyst volume was assumed to equal 1.5 times the engine swept volume, or 7.5 liters. Additional inputs values used are contained in Table 2.

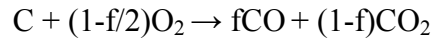
Table 2: SCR Input Values

Monolith Diameter	0.1524 m
Monolith Length	0.41 m
Number of Cells Per Square Inch	200
Cell Hydraulic Radius	0.00072 m
Monolith Void Fraction	0.647

DPF Model

As discussed above, an active (catalyzed) DPF was chosen due to the low engine out exhaust temperature of this application. Once the filter reaches capacity, a deliberate addition of energy is required for filter regeneration. While this energy addition can take various forms, such as direct electrical or microwave heating, we assume that fuel addition upstream of the filter provides heat for regeneration.

Therefore, the reaction set for the DPF is:



The quantity "f" represents the thermal CO selectivity for carbon oxidation. This value was set at 0.1 for this analysis. The reaction rate mechanism used for this reaction is:

$$R_1 = A_1 e^{-B_1/T} [C][O_2]$$

The exponential constant of this equation was set to a value given in Konstandopoulos, Kostoglou, Skaperdas, Papaioannou, Zarvalis, and Kladopoulou (5). The pre-exponential constant was tuned to internal data.

The model used the pressure drop methodology developed by Konstandopoulos et al (5). Input values for the model are based either on this source or from experience and are presented in Table 3.

Table 3: DPF Input Values

Particulate density	80 kg/m ³
Particulate permeability	0.25 X 10 ⁻¹⁴ m ²
Filter wall pore diameter	9.0 x 10 ⁻⁶ m
Filter wall thickness	2.79 x 10 ⁻⁴ m
Filter wall permeability	0.5 x 10 ⁻¹³ m ²
Filter Diameter	0.1524 m
Filter Length	0.41 m
Number of Cells Per Square Inch	300
Cell Hydraulic Radius	0.00059 m
Monolith Void Fraction	0.655

While Konstandopoulos et al (5) provides a transient filtration model based on “unit collector” filtration theory, the use of such a model is outside the scope of this study. A look up table of filtration efficiency versus filter loading using the values presented in Table 4 is used instead.

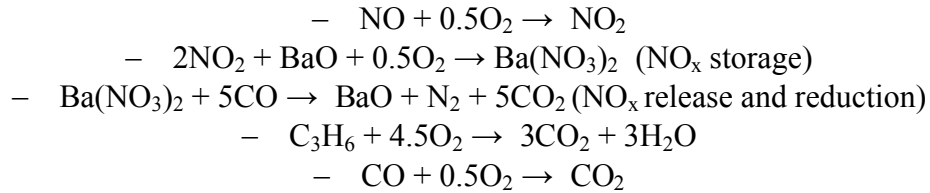
Table 4: DPF Filtration Efficiency Versus Soot Loading

Carbon Loading (kg)	Filtration Efficiency (%)
0	85
0.0016	94
0.0032	99
0.0065	99
0.01	99

Once the filter reaches its capacity of 40 grams, regeneration is achieved by heating the exhaust entering the DPF to 600°C and maintaining this temperature until the filter reaches 5 grams of particulate or less. (The reaction will continue for some time after heat is removed, but the cooler exhaust eventually cools the filter to below light off temperature.) For exhaust conditions during regeneration, an average speed/load point from the FTP was chosen.

NAC Model

For this study, the NAC model assumes barium oxide (BaO) chemistry. CO is assumed to be the only reductant. While other reductants and/or storage species are discussed in literature, lack of appropriate data necessitated these assumptions. Tuning an NAC requires detailed transient data of both inlet and outlet species over both the rich and lean cycles as well as other test variables such as monolith temperature and catalyst details such as NO_x capacity. Even with this data, an NAC is difficult to tune due to lack of information concerning the status of BaO and Ba(NO₃)₂. Since data with sufficient detail was unavailable, a simplified reaction set was used. This reaction set is shown below.



As can be seen from the reaction set, the storage and reduction reactions have been combined into one reaction, which made tuning possible with the available data. The following rate mechanisms were used:

$$R_1 = \frac{A_1 e^{-B_1/T} [NO][O_2]}{(1 + C_1 e^{-D_1/T} [O_2]^{0.5} + E_1 e^{-F_1/T} [NO])^2} \quad (1)$$

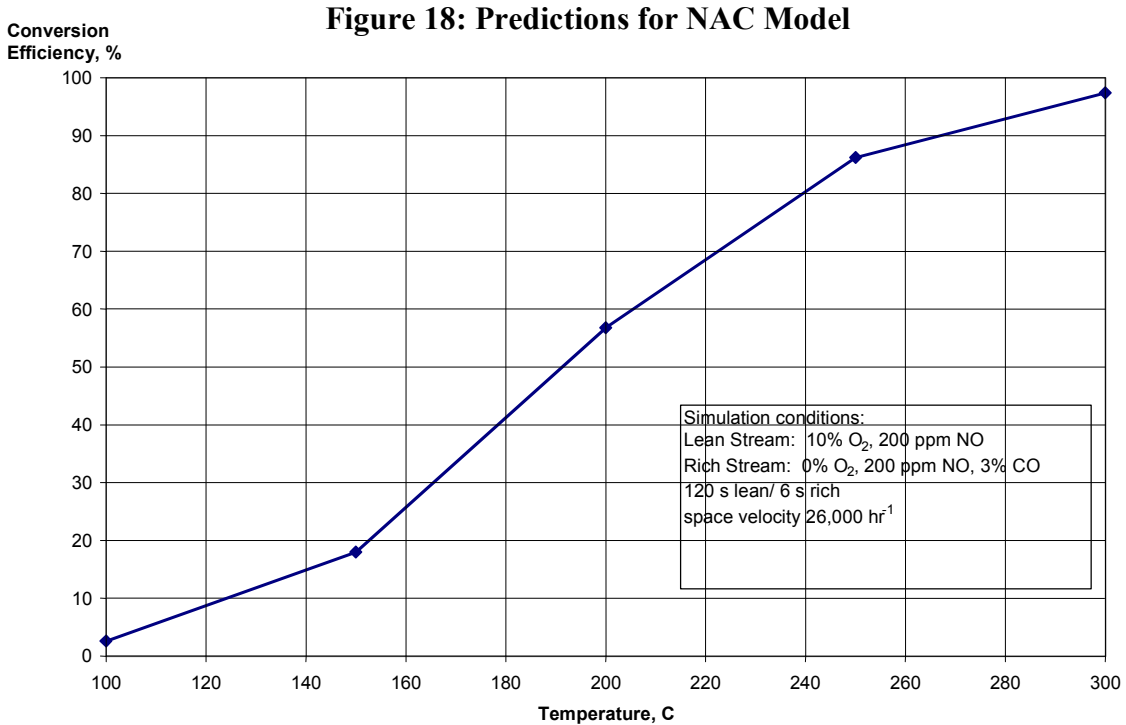
$$R_2 = A_2 e^{-B_2/T} [BaO][NO_2] \quad (2)$$

$$R_3 = A_3 e^{-B_3/T} [Ba(NO_3)_2][CO_2] \quad (3)$$

$$R_4 = \frac{A_4 e^{-B_4/T} [C_3H_6][O_2]}{T_s (1 + K_1[CO] + K_2[C_3H_6])^2 (1 + K_3[CO]^2 [C_3H_6]^2) (1 + K_4[NO]^{0.7})} \quad (4)$$

$$R_5 = \frac{A_5 e^{-B_5/T} [CO][O_2]}{T_s (1 + K_1[CO] + K_2[C_3H_6])^2 (1 + K_3[CO]^2 [C_3H_6]^2) (1 + K_4[NO]^{0.7})} \quad (5)$$

Rate equations 1, 4, and 5 are from Shamim, Shen, and Sengupta (6). The constants for reaction 4 and 5 were taken from that reference as well. The rest of the reactions were tuned to approximate internal performance data. Figure 18 shows the results of this tuning.



The activation energy for reactions 2 and 3 were adjusted to allow some adsorption at lower temperatures while release/reduction was kept above 180-200°C. This is consistent with NREL's experience. Performance tests indicate that NAC NO_x storage capacity decreases with decreasing temperature. The modeled NAC, however, is large enough

with respect to the engine out stream so that this was not considered an issue; therefore, the modeled NAC assumes a constant NO_x storage capacity regardless of temperature.

For this application, the catalyst volume was assumed to be 5.1 liters with a 2 g/L NO_x capacity. With the engine producing approximately 3.3 g NO_x over an FTP, the maximum fill of a clean NAC over the FTP is 33%. Other inputs used are presented in Table 5.

Table 5: NAC Input Values

Monolith Diameter	0.1524 m
Monolith Length	0.2794 m
Number of Cells Per Square Inch	400
Cell Hydraulic Radius	0.00055 m
Monolith Void Fraction	0.76

While regeneration strategy is crucial to obtaining good conversion efficiencies, the low engine out temperature in this application is the main inhibitor of performance. Therefore, a simplified regeneration strategy was pursued—regenerations are scheduled for 6 seconds of duration with 120 seconds of lean operation in between. If the average monolith temperature is less than 180°C at the scheduled time, the regeneration is not initiated. The next possible regeneration is 126 seconds later.

LNC Model

The original intent of this study was to model the NAC, SCR, and DPF, while estimating the performance of the LNC. The actual path taken was to model the LNC in a more simplistic fashion than for the NAC or SCR. The model was amended to accept a conversion efficiency map in lieu of the diffusion and reaction submodels. The thermal model was kept intact, and reaction enthalpy is accounted for. This modified approach provides an accurate temperature history of the monolith, which will result in a better prediction than an estimate based just on engine out temperature. Furthermore, this approach makes LNC performance versus time over the FTP available for direct comparison with the other simulations.

The LNC assumes propene addition to convert NO_x over platinum on alumina (Al₂O₃) catalyst; this was used as a surrogate for diesel fuel to simplify the reaction mechanism. The peak performance of the LNC resulted in a NO_x conversion efficiency of approximately 85% at 220°C. This data was obtained for a C/ NO_x ratio of 8:1, so additional propene was added (in a similar fashion to urea) for SCR.

Platinum on alumina catalysts can show a high propensity for nitrous oxide (N₂O) formation. On some catalysts the N₂/N₂O ratio in the exit stream can be 50% or greater. For the purposes of this study, however, N₂O formation is not predicted. All NO_x converted is assumed to produce N₂ only.

Hydrocarbon injection was enabled whenever the average monolith temperature was greater than 150°C. This was done because in a real application, hydrocarbon injection under this temperature could cause the formation of organic deposits on the catalyst surface that could degrade performance.

Emissions Modeling Results

All calculations on a per mile basis use an FTP length of 11.04 miles. Diesel fuel density is assumed to be 850 g/liter, and the lower heating value is assumed to be 43,000 J/g. Data for diesel fuel were taken from ADVISOR.

SCR/DPF System

Table 6 shows tailpipe emissions and fuel economy results for each of the technology bundles. The tailpipe emissions from the SCR/DPF system equate to 0.13 g/mile NO_x and 0.0077 g/mile PM (for an empty DPF; 0.0057 g/mile when the DPF is full). Therefore, the vehicle would qualify for Tier 2 bin 8. The attendant fuel economy reduction, as shown in Table 6, is 0.38% with a perfectly clean DPF and 1.14% when the DPF is full. Table 7 shows the reduction in emissions, increase in fuel consumption, and the ratio of fuel consumption increase to emissions reduction for the three technology bundles. The grams of fuel used/grams of emissions avoided for the SCR/DPF system is 2.0 for a clean DPF and 6.1 for a full DPF. Figure 19 graphically depicts these values for each technology bundle. As can be seen the SCR/DPF system as well as the other two systems fail to meet the Tier 2 bin 5 goals for NO_x. All of these systems will need additional modification to achieve the Tier 2 bin 5 goal.

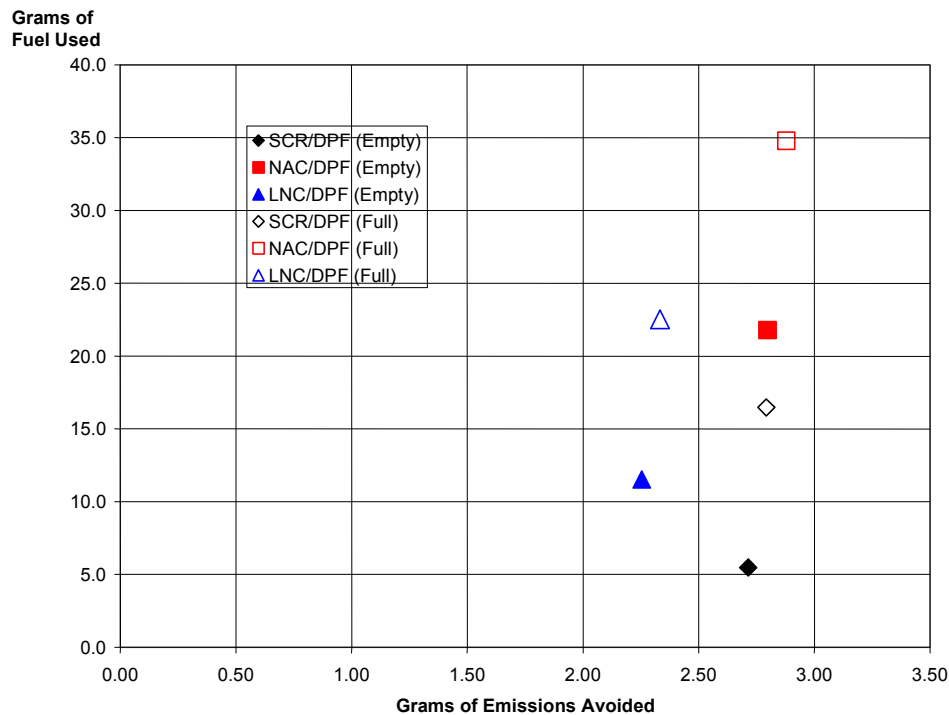
Table 6: Simulation Results In Terms of Grams Per Mile and Miles Per Gallon

	Baseline	SCR + DPF	NAC + DPF	LNC+DPF
NO _x (g/mile)	0.32	0.13	0.12	0.17
PM (g/mile) Empty DPF/Full DPF	0.057	0.0077/0.0057	0.0079/0.0059	0.0077/0.0057
Fuel Economy (mpg) Empty DPF/Full DPF	24.6	24.5/24.4	24.3/24.1	24.4/24.3
Tier 2 Emissions Bin	10	8	8	9
Fuel Economy Penalty Empty DPF/Full DPF	N/A	0.38%/1.14%	1.51%/2.41%	0.80%/1.56%

Table 7: Simulation Results In Terms of Grams of Emissions Avoided and Grams of Fuel Used

	NO _x Reduction (g)	Pm Reduction (g) Empty DPF / Full DPF	Total Emission Reduction (g) Empty DPF / Full DPF	Fuel Economy Penalty (g) Empty DPF / Full DPF	Grams of Fuel Used / Grams of Emissions Avoided Empty DPF / Full DPF
SCR+DPF	2.17	0.544/0.623	2.71/2.79	5.5/16.5	2.0/6.1
NAC+DPF	2.26	0.541/0.622	2.80/2.88	21.8/34.8	7.8/12.4
LNC+DPF	1.71	0.544/0.623	2.25/2.33	11.5/22.5	5.1/10.0

Figure 19: Grams of Fuel Used Versus Grams of Emissions Avoided



The cumulative NO_x conversion efficiency for SCR is 61% over the FTP. NO_x conversion for both SCR and NAC starts at approximately 60 seconds, while significant conversion starts at about 180 seconds. Pure urea usage over the FTP is 2.63 grams. The primary reason for the poor NO_x conversion is low engine out exhaust temperature. As discussed previously, the urea injection is enabled only for exhaust temperatures greater than 180°C to avoid partial conversion to ammonia and the potentially harmful byproducts that may form. While a hot surface will promote urea conversion, Figure 20 shows that the average monolith temperature of SCR over the FTP cycle rarely exceeds 180°C. Therefore, limiting urea injection, in conjunction with low ammonia storage capacity, severely limits NO_x conversion.

The injection of ammonia (rather than urea) could overcome this limitation, and could potentially increase the conversion efficiency from the current 59% to 70% or more. The problems associated with the handling of storage ammonia prevent this from being a possibility.

Figure 21 shows the particulate emissions over the FTP for a clean DPF. The average filtration efficiency over the FTP is 86.5%. As discussed earlier, filtration efficiency will improve to a value of 99% with increasing filter soot loading.

Figure 22 illustrates the regeneration of the DPF from steady state conditions corresponding to the average FTP engine speed and load. The DPF is assumed to contain 40 grams (filter capacity) of soot at the start of simulation. The DPF required 612 seconds of 600°C exhaust gas to regenerate to 3.7 grams of soot. The average engine speed and load during the FTP are 1200 rpm and 52 Nm, which yields an exhaust temperature of 140°C and an exhaust mass flow rate of 0.02 kg/s. Assuming an exhaust specific heat of 1089 J/kg-K and a LHV of 43,000 J/g, this equates to 143 grams of fuel. The DPF will fill over approximately 60 FTP cycles. Therefore, the regeneration fuel usage spread out over the 60 cycles is 2.38 grams. This value is taken into account in Tables 6 and 7 as well as Figure 19.

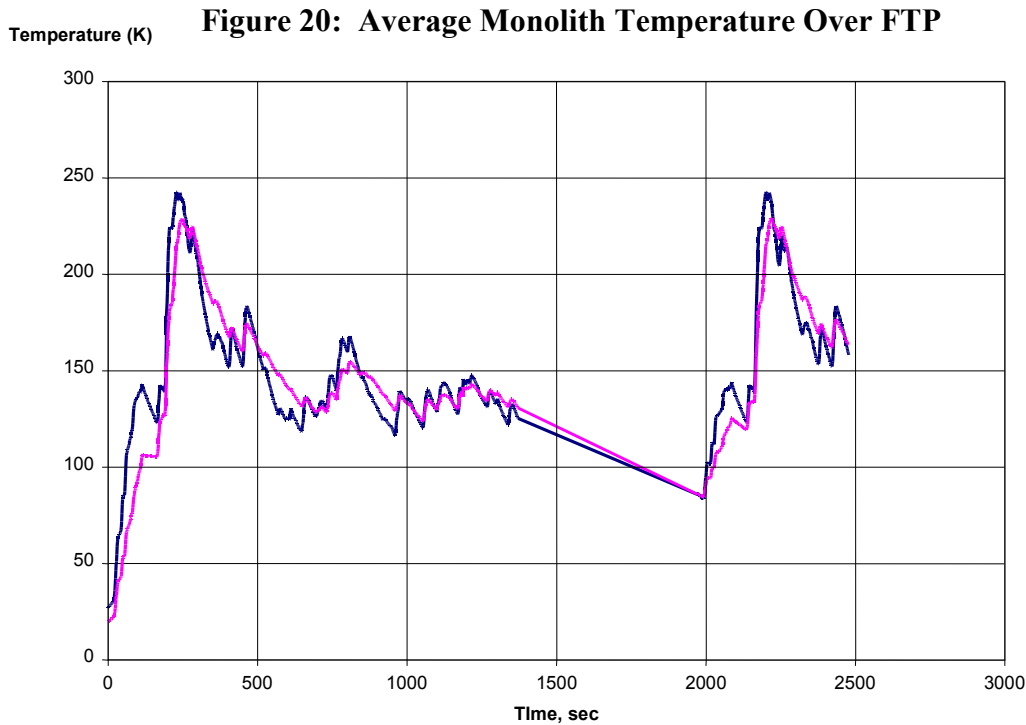


Figure 21: DPF Soot Reduction Performance

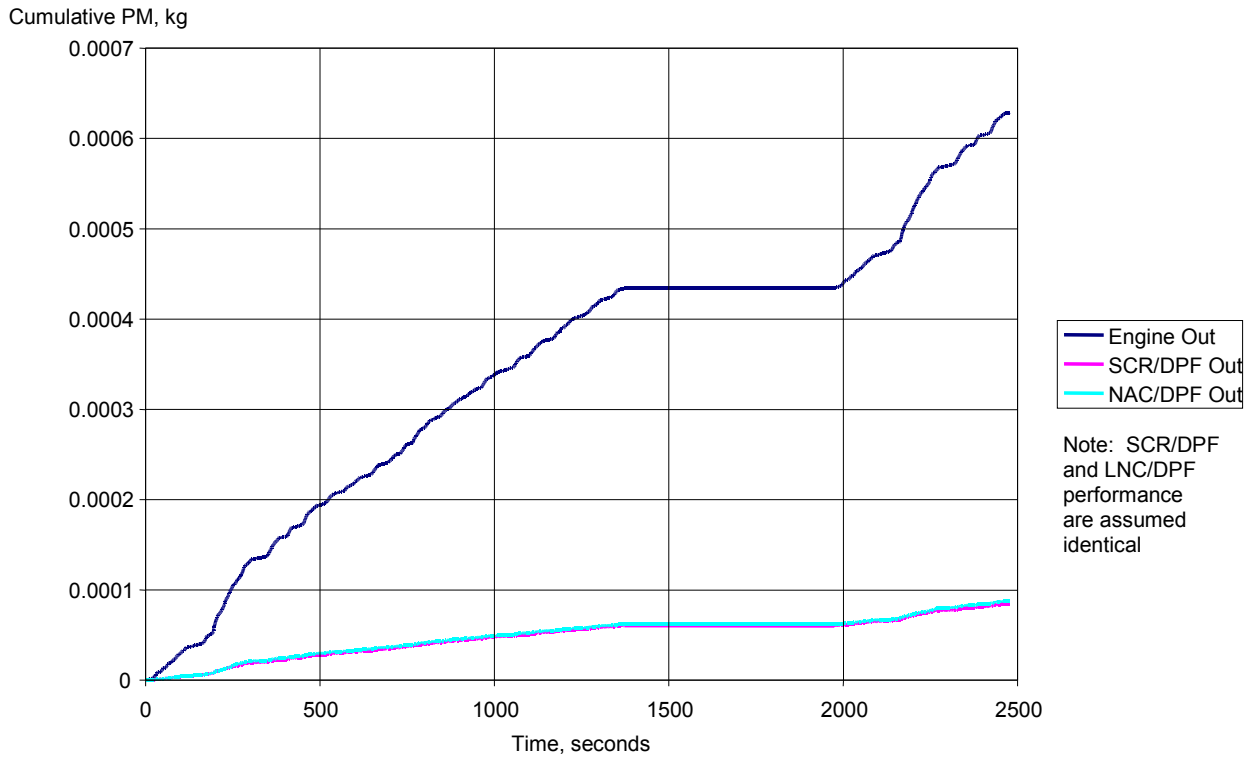
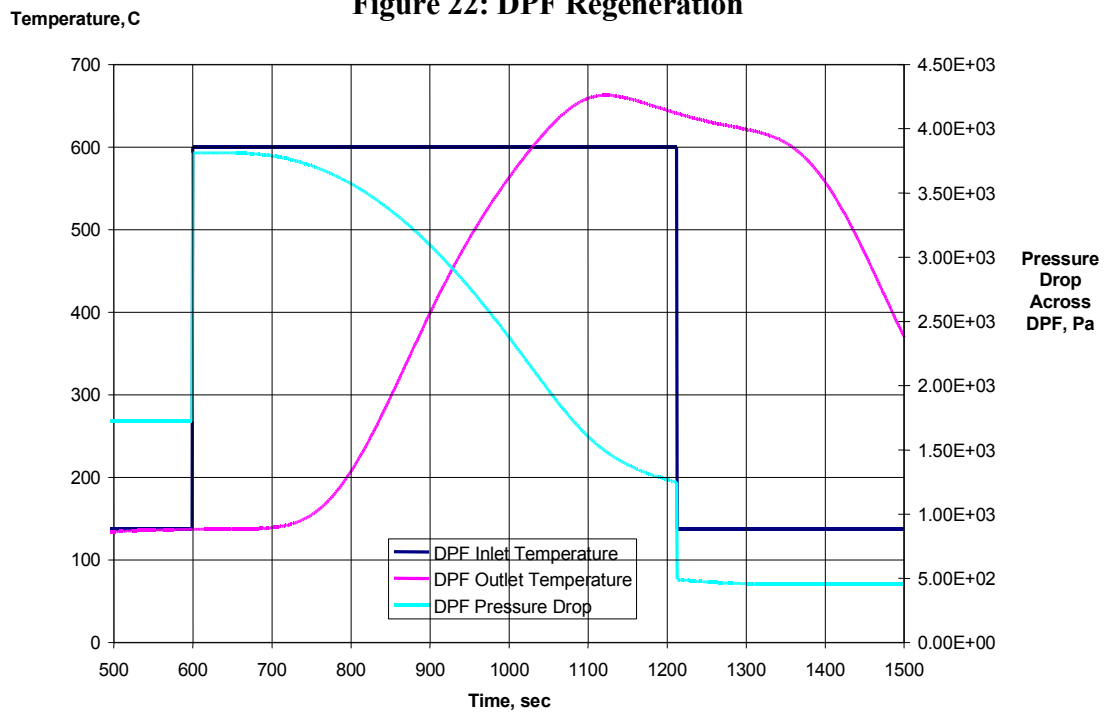


Figure 22: DPF Regeneration



The fuel penalty for this application is very small. However, the effect of backpressure at low engine speed and loads is small. This is not the case at higher engine speeds and loads.

NAC/DPF System

Table 6 shows that the tailpipe emissions from the NAC/DPF system equate to 0.12 g/mile NO_x and 0.0079 g/mile PM (for an empty DPF; 0.0059 g/mile when the DPF is full). Therefore, the vehicle would qualify for Tier 2 bin 8. The attendant fuel economy reduction, as shown in Table 6, is 1.51% with a perfectly clean DPF and 2.41% when the DPF is full. Table 7 shows that the ratio of grams of fuel used to grams of emissions avoided is 7.8 for a clean DPF and 12.4 for a full DPF. Figure 19 graphically depicts these values.

Cumulative NO_x conversion efficiency for the NAC is 63% over the FTP. NO_x conversion for both SCR and NAC starts at approximately 60 seconds, while significant conversion starts at about 180 seconds. Once again, low engine out exhaust temperature is the main reason for low conversion efficiency.

Due to the limit of NAC regeneration to average monolith temperatures of 180°C and above, only two six-second regenerations are made during the FTP. The average monolith temperature over the FTP is shown in Figure 19. One of the regenerations occurs at 246 seconds and the other at 2262 seconds. The trap attains a maximum of 15% fill during the FTP, and the fill at the end of the FTP is approximately 9%. A simulation of a second FTP with initial conditions based on the end of the first FTP does not show any appreciable increase in emissions or final trap fill.

The rich spikes decrease engine out NO_x while increasing engine out PM. This is why the DPF, which is identical between SCR and NAC systems, has greater tailpipe PM emissions than the NAC system. The filtration efficiency for the DPF with the NAC is 86.1%, which can barely be seen in Figure 20.

LNC/DPF System

Table 6 shows that the tailpipe emissions from the LNC/DPF system equate to 0.17 g/mile NO_x and 0.0077 g/mile PM (for an empty DPF; 0.0057 g/mile when the DPF is full). Therefore, the vehicle would qualify for Tier 2 bin 9. The attendant fuel economy reduction, as shown in Table 6, is 0.80% with a perfectly clean DPF and 1.56% when the DPF is full. Table 6 shows that the ratio of grams of fuel used to grams of emissions avoided is 5.1 for a clean DPF and 10.0 for a full DPF. Figure 7 graphically depicts these values.

Cumulative NO_x conversion efficiency for the LNC is 48% over the FTP. NO_x conversion starts at approximately 200 seconds, which is due to the higher light off temperature of the LNC. The poor performance, therefore, is due to the low exhaust

temperature in conjunction with the LNC having a higher light off temperature and a lower maximum conversion efficiency than either SCR or the NAC.

Soot increase resulting from the HC injection required for NO_x reduction in the LNC was assumed negligible. Therefore, the DPF inlet stream is identical to that of SCR, and since the DPF is an active type, the performance of the DPF with the LNC is identical to the DPF with SCR.

Comparison of the Technology Bundles

Tables 6 and 7 and Figure 19 provide a comparison of the performance of the three emissions control technology bundles. In regard to tailpipe NO_x emissions, the NAC at 0.12 g/mile is slightly better than SCR at 0.13 g/mile. The LNC is far behind SCR and NAC at 0.17 g/mile. All three fall far short of the Tier 2 bin 5 goal of 0.05 g/mile— SCR and NAC achieve bin 8, while the LNC achieves bin 9. SCR, NAC, and LNC, which provided 61%, 63%, and 48% conversion efficiency, respectively, over the FTP, would have to reach 84% conversion efficiency over the FTP to make bin 5. This represents a 38%, 33%, and 75% increase in performance for SCR, NAC, and LNC, respectively, to meet Tier 2 bin 5. Additional exhaust systems modifications (e.g. catalyst close coupling), thermal generation or management strategies, and engine management strategies (e.g. aggressive EGR) for these applications should result in achieving the Tier 2 bin 5 NO_x goal.

For all three bundles, PM emissions are not a concern—the limiting emissions are NO_x. The same DPF was used in each bundle, so tailpipe results between the three bundles are very close. The NAC had the worst performance at 0.0079 g/mile due to the rich spikes increasing engine out PM emissions,. SCR and LNC bundles posted 0.0077 g/mile. Bins 2 through 6 have a PM limit of 0.01 g/mile. It should be noted that the tailpipe PM emissions stated are for a clean filter, and the filter efficiency increases with soot loading. The trapping efficiency of the DPF is improved with some soot loading.

The emissions reductions come with an attendant fuel penalty of up to 2.41% for the NAC, 1.56% for the LNC, and 1.14 % for SCR. This penalty is due to increased backpressure from the catalyst and DPF, additional fuel required for rich-spike regeneration of the NAC, hydrocarbon injection for LNC operation, and fuel necessary for DPF regeneration spread over the number of cycles necessary to fill the filter. Other factors, such as fuel required for NAC desulfation were not included. With the zero sulfur fuel assumed in this study, NAC desulfation events should have a minor additional impact on NAC fuel penalty. The impact on fuel consumption penalty is possibly similar to that of the DPF regeneration, raising the NAC fuel penalty from 2.41% to 2.61%.

Reaching higher conversion efficiencies for all three technologies could be achieved by maintaining the exhaust gas temperature at some minimum value using fuel injection into the exhaust gas stream. Urea injection, regeneration of the NAC, and injection of fuel for the LNC were all limited at low catalyst or engine out exhaust gas temperatures. Therefore, raising the exhaust gas temperature would increase urea usage or fuel usage

over the values calculated by simulation. The amount of increase is difficult to determine, but may reach 5% or more for the NAC, and 4.5% or more for the LNC. Urea usage for SCR may increase four fold or more. Additional analysis would be necessary to refine these estimates.

SCR urea usage over one FTP cycle was 2.63 grams. This would require 7.57 grams of 35% wt urea solution that is proposed for distribution. Assuming a 2:1 ratio of fuel to reductant costs per volume, and a specific gravity of diesel fuel of 0.85, the financial penalty due to SCR consumption would be the equivalent of raising the fuel penalty from 1.14% to 1.5%.

When fuel economy versus emissions reduction is taken into consideration, SCR at 6.1 grams of fuel used per gram of emissions avoided is clearly more efficient than the NAC at 12.4 and the LNC at 10.0. This is somewhat misleading, however, since the LNC is much lower in conversion efficiency than both the NAC and SCR.

Summary of Emissions Modeling Results

- A 5.0-liter diesel engine in a mid-sized SUV is very lightly loaded over the light-duty FTP cycle. The resulting turbine out exhaust temperature is extremely low for currently reported catalysts. This leads to lower conversion efficiencies. To alleviate this problem, smaller, more highly loaded engines should be considered.
- The NAC and SCR systems attain Tier 2 Bin 8 emissions standards with maximum fuel consumption increases of 1.14% and 2.4%, respectively. The LNC system attains Tier 2 Bin 9 emissions with a fuel consumption increase of 1.56%. In terms of grams of fuel used per gram of emissions avoided, SCR at 6.1 is clearly more efficient than the NAC at 12.4 and the LNC at 10.0.
- In all cases, the NO_x emissions are limiting; PM emissions for all three systems qualify for Tier 2 Bin 2.

5 FUTURE DIRECTION

In FY 2003 activity will continue to focus on the three APBF platforms: a light-duty passenger car, light-duty truck/SUV, and a heavy-duty engine. For these platforms, activity will be focused on the following areas:

- Continue to build SER analysis capabilities:
 - Apply 1-D engine models developed in FY 2002 to evaluate various aspects of emission control technology on fuel economy and engine performance. Specifically, 1-D engine models can be employed to understand the impacts of factors such as engine back pressure, friction, injection timing, EGR ratio, and others on fuel economy and emissions.
 - Incorporate a heavy-duty engine model in to ADVISOR
- Build on industry relationships in order to maximize opportunities for collaboration.
- Continue modeling of emission and fuel penalty trade-offs
 - Evaluate the emission reduction and fuel economy trade-offs for promising CIDI NO_x emission control technologies for the heavy-duty passenger car platforms.
 - Investigate raising the exhaust gas temperature—Methods such as turbocharger bypass, hydrocarbon injection into the exhaust gas stream, strategic reduction in EGR cooling, and cylinder deactivation would raise the exhaust gas temperature and could increase conversion efficiencies.
 - Evaluate mild hybridization—A mild hybrid would allow regenerative braking and enable electric heating of the filter or the exhaust gas stream, thus increasing conversion efficiency. For an SCR system, the electrical energy could be used to assist in converting urea to ammonia, which would extend the low temperature operation of SCR.
 - Consider a NO_x occluding system—Investigate a system capable of storing (via physisorption, as opposed to chemisorption, as with the NAC) NO_x at low temperatures and reinjecting the NO_x back into the exhaust stream once a NO_x catalyst—LNC, SCR, or NAC—reaches its lightoff temperature.
 - Downsize engine for SUV platform—A smaller, more highly loaded engine will have higher exhaust temperatures, which will lead to higher conversion efficiencies. Engine out emissions may be higher, however.

The project will also evaluate applications related to all vehicle platforms as necessitated by DOE and the needs of the APBF-DEC activity. The SER analysis will provide DOE with predictions regarding the potential effectiveness of different combinations of fuel, CIDI engine control strategies, and emission control devices, for meeting emission reduction targets and engine and vehicle performance goals. These activities will support evaluation of the best pathways for achieving the technical targets of the overall APBF-DEC activity and better understand of the emissions and fuel economy trade-offs between various lean exhaust NO_x emissions control devices such as NO_x adsorbers, selective catalytic reduction, and non-thermal plasma.

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